1,4-Naphthoquinone 130-15-4 | DTXSID5040704

Model Performance

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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 8.12 days

Global applicability domain: Outside

Local applicability domain index: 4.54e-01

Confidence level: 8.01e-01

Nearest Neighbors from the Training Set

Image not found

Ethylbenzene Measured: 120 Predicted: 6.21 Image not found

1,3-Diethylbenzene Measured: 88.3 Predicted: 5.36 Image not found

4-Phenyltoluene Measured: 4340 Predicted: 25.1

Image not found

Propylbenzene Measured: 24.3 Predicted: 4.02 Image not found

4-Ethyltoluene Measured: 24.3 Predicted: 3.95